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KNOT INVARIANTS AND CELLULAR AUTOMATA

N00014-91-J-1512

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1. Introduction

The goal of this project was to build on an understanding of the connections between knot invariants, exactly solvable statistical mechanics models and discrete dynamical systems toward an answer to the question of how early and robust thermodynamic behavior appears in lattice gas automata. Preliminary work focussed on developing our understanding of state models in knot theory and their relation to statistical mechanics models; this work is described in [1].

Rather than considering the complicated and somewhat more difficult case of lattice gas hydrodynamics we began with a simpler model: a reversible cellular automaton in one dimension. This particular automaton has an additive conserved quantity which Takesue has used to construct a one dimensional statistical mechanics model [2]. He observes in simulations that the cellular automaton displays thermodynamic behavior which is well described by this one dimensional statistical mechanics model. In [3] and [4] we showed that there is a naturally associated two dimensional statistical mechanics model as well, then examined the properties of this model, and suggested how these properties may relate to the behavior of the dynamical cellular automaton. This work is described in the following section.

Having applied these ideas successfully to the simple case of a reversible cellular automaton, we moved on to the more interesting case of lattice gases. Since our approach equates the spacetime evolution of a dynamical system with an equilibrium configuration of a statistical mechanics model in one higher dimension, a model of 't Hooft for two dimensional spacetime with discrete local coordinate invariance was a natural inspiration [5]. In [6] we detail the construction of a family of one dimensional lattice gas automata based on this model. This work is summarized in section 3.

2. Cellular automata

We focus on reversible models for several reasons: Microscopically, one expects physical theories to be reversible. Moreover, with the additional constraint of discreteness, reversibility implies that phase space volume is conserved under the evolution; hence an analog of Liouville's Theorem applies. Finally, when some locally defined and additive quantity is conserved, the system is similar to a Hamiltonian system, the context in which questions of ergodicity and thermodynamic behavior are usually studied.

Motivated by these considerations, Takesue has begun an analysis of the class of one dimensional reversible cellular automata with a nearest neighbor rule [7]. In particular, consider the the one dimensional automaton with a boolean variable at each site evolving according to

$$\sigma_i^{t+1} := f(\sigma_{i-1}^t, \sigma_i^t, \sigma_{i+1}^t) \text{ XOR } \sigma_i^{t-1}$$

where $f : \{0,1\}^3 \longrightarrow \{0,1\}$ is given by

$$f(\lambda, \mu, \nu) := \lambda + \nu - \mu\nu - 2\lambda\nu + \lambda\mu\nu,$$

rule 26R in the usual conventions [8]. There is a conserved quantity defined by

$$E := \sum_i E(\sigma_i^{t-1}, \sigma_{i+1}^{t-1}, \sigma_i^t, \sigma_{i+1}^t) := \sum_i \left[(\sigma_i^t - \sigma_{i+1}^{t-1})^2 + (\sigma_{i+1}^t - \sigma_i^{t-1})^2\right].$$

Takesue uses this result in one test of thermodynamic behavior [2]: Any initial configuration has some total energy which determines an inverse temperature β. In simulations he observes a canonical ensemble at this temperature for subsystems. More precisely, the dynamical distribution of energies E_n for a subsystem of size $n+1$ is found to be close to $D(E_n)\epsilon^{-\beta E_n}$ where $D(E_n) := (\textit{number of configurations with energy } E_n)/4^{n+1}$. This phenomenon is observed even for fairly small values of N and n. Similarly, he finds that by simulating a heat bath at either end of the system, rule 26R supports a temperature gradient [9].

Thus this automaton exhibits the type of surprising thermodynamic behavior we would like to understand: Despite being far from the thermodynamic limit (small N and n) the dynamical system displays equilibrium behavior well approximated by this statistical mechanics model. Moreover, such success suggests that the system is ergodic. We know, however, that it cannot be truly ergodic, for there are $O(2^N)$ cycles [7] and only $2N$ energy surfaces, which means that the energy surfaces must be partitioned into many orbits.

Our suggestion is that the origin of this thermodynamic behavior might be found in a naturally associated two dimensional statistical mechanics model. The Boltzmann weight $W_{cd}^{ab} := \exp[-\beta E(a,b,c,d)]$ can be identified as the transition

matrix for the scattering process $(\sigma_i^{t-1}, \sigma_{i+1}^{t-1}) \longrightarrow (\sigma_i^t, \sigma_{i+1}^t)$ or, equally well, as the Boltzmann weight of a vertex model on a square lattice. Thus the deterministic dynamical evolution of the cellular automaton is modelled probabilistically (hence not exactly) by two such statistical mechanics models on a pair of dual lattices

Now, recall the transfer matrix method for the solution of two dimensional statistical mechanics models [10]. For the model we are considering here the partition function is

$$Z := \sum_{\text{states}} \prod_{\text{vertices } i} e^{-\beta E_i},$$

where the energy E_i associated to a vertex i is determined by evaluating the expression for the conserved quantity above on the spins (boolean values) assigned to the incident edges by a given state. To apply the transfer matrix method to this model we would proceed by defining the diagonal-to-diagonal transfer matrices and find that the partition function again becomes the trace over a product of identical matrices.

Thus the problem of solving this model in the thermodynamic limit reduces to the problem of determining the largest eigenvalue of some $2^N \times 2^N$ transfer matrix T. Because commuting matrices have common eigenvectors it has proved sufficient in models like this one to recognize T as an element in a one parameter family $T(\omega)$ of mutually commuting transfer matrices: $[T(\omega), T(\omega')] = 0$, where the spectral parameter ω is determined by the coupling constants/interaction strengths in the energy functional defining the model. Further, it is easy to see that a sufficient condition for the existence of commuting transfer matrices is that the Boltzmann weights satisfy the Yang-Baxter (star-triangle) equation [10,11]:

$$W_{ij}^{ab}(\omega) W_{kf}^{jc}(\omega + \omega') W_{de}^{ik}(\omega') = W_{ki}^{bc}(\omega') W_{dj}^{ak}(\omega + \omega') W_{\epsilon f}^{ji}(\omega).$$

The relevance of this result to our problem is the following. The two component (spin $\frac{1}{2}$) solutions to the Yang-Baxter equation have been classified. The most general solution is the eight-vertex model in which the Boltzmann weights are parameterized by elliptic theta functions [12]. In this model the temperature is related to the theta function nome p in such a way that $p = 0$ corresponds to $T = T_{\text{critical}}$. Moreover, only at $p = 0$ is the limit $\omega \to \infty$ defined. In this limit one obtains the six-vertex model and the Yang-Baxter equation becomes independent of the spectral parameter:

$$W_{ij}^{ab} W_{kf}^{jc} W_{de}^{ik} = W_{ki}^{bc} W_{dj}^{ak} W_{\epsilon f}^{ji}.$$

This is precisely the condition realizing the type III Reidemeister move of knot theory [11,13] and is, as we showed in [3], satisfied by the Boltzmann weights of our two dimensional statistical mechanics model. Thus our cellular automaton is really the (critical) six-vertex model in disguise.

Now, the dominant characteristic of criticality is scale or conformal invariance, which means that probability distributions of states are invariant and correlation functions transform covariantly under conformal transformations. Thus, if our model were really at a critical point, i.e., $N \to \infty$ as well as $T = T_{\text{critical}}$, the local distribution of states would be that of the thermodynamic limit, a result consistent with an observed canonical distribution. For finite N this will be moderated by finite-size effects which round off the critical singularity. Some finite-size effects can be computed explicitly [14]; for example, the correlation length will be asymptotically proportional to N. This, in fact, is exactly what Takesue observes when he measures the autocorrelation function of the energy flux to check the Green-Kubo formula [9]. So the criticality of the associated two dimensional statistical mechanics model is nicely consistent with the observed thermodynamic behavior of the cellular automaton.

3. Lattice gases

Moving on to the simplest type of lattice gas model, in [6] we described the construction of a family of one dimensional lattice gas automata based on a model of 't Hooft [5]. In an effort to clarify which features of the lattice gas automata are the consequences of which constraints, we proceeded systematically: first setting the kinematics of the model, then exploring the effect of requiring that the dynamics be local, and finally constructing the possible dynamics consistent with the imposed constraints.

The most interesting of these three steps is the second. By *local* dynamics we mean that two particles interact only when they coincide in both space and time. The simplest consequence of this requirement is illustrated in Figure 1. There particles 1 and 2 interact at time $t + 1$, but particles $1'$ and 3 move past each other without interacting because their spatial coordinates always differ by an odd number, precluding coincidence. This apparently trivial observation is at the origin of the "spurious" conserved quantities often found in lattice gas models: here the gas decouples into two noninteracting gases, one occupying the even nodes of the lattice and the other the odd. In [3] and [4] we used the conserved quantity of the cellular automaton to define the weights of the equivalent statistical mechanics model. Here, rather than follow the usual approach to dealing with a spurious conserved quantity (modifying the model in an attempt to break the unwanted conservation law) we use it to effect a radical transformation of the model to one which is again equivalent to a 2 dimensional statistical mechanics model. The transformation is described in [6]; to our knowledge this is the first time such an approach has been taken.

The conclusion is that the model lies on a first order critical line between disordered and totally ordered regimes of the six vertex model. We observe that this result applies to ensembles of systems, in the thermodynamic limit. That the correlation length vanishes, for example, does not mean that there is no correlation

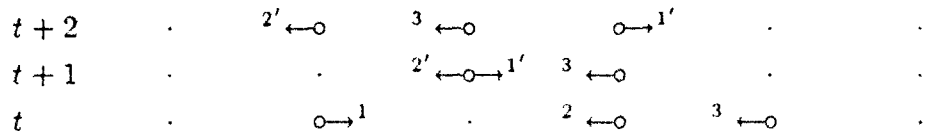

Figure 1.

between states of the probabilistic lattice gas automaton at successive time steps. Nor would a nonvanishing correlation length mean that there were necessarily spacelike correlations in a given initial state. Instead, the interpretation is that deep in the interior of a system, far from the boundary conditions and thus/or subject to essentially random boundary conditions, a domain of sufficiently large size is in thermodynamic equilibrium. Thus our results provide evidence for the first step in the derivation of the macroscopic equations of motion—the assumption of local thermodynamic equilibrium, as well as demonstrating the efficacy of constructing and analyzing lattice gas automata according to (spacetime) symmetry principles.

In 't Hooft's original model the particle trajectories were to be interpreted as defect lines in a (spacetime) lattice which developed curvature at the crossing (interaction) points. Our immediate concern then, at least for this model, is to determine the consequences for this interpretation of our transformation to a solvable statistical mechanics model and the conclusions about its thermodynamics that we thereby draw. Our results should be compared to a model where the energy of a configuration depends on the curvature as it does both in models for spacetime and models for crystalline materials. Of course, this also raises the general question of what energies/weights might be appropriate when such a simple lattice structure is not available. For an interacting particle model of a generic dynamical system the weakest information to which one would have access is the causal ordering of the interactions; our work to this point suggests addressing the question of whether at least some such models could be mapped into a statistical mechanics framework: though one could not expect the resulting model to be solvable, some understanding of the dynamical system might be gained nevertheless.

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